Scientific Python Introduction

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Materials Physics Center
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Why Python?

```
print("Hello, world!")
```

Why Python?

Python is inherently slow compared to C/C++ or FORTRAN, so why Python for Scientfic Computing?

Python is slow, but...

Syntactically, Python code looks like executable pseudo code. Program development using Python is 5-10 times faster than using C/C++...

The best approach is often to write only the performance-critical parts of the application in C++ or Java, and use Python for all higher-level control and customization.

– Guido van Rossum

Why Python?

We have (for free)

- A general purpose language with a huge spectrum of freely available libraries for almost anything you can think of.
- A very easy to learn (and read) language that smoothly interfaces with C/C++ and FORTRAN (eg. calculation kernels).
- Lots of wrappers for well stablished, fast and long time tested numerical packages.
- Lots of high level utility libraries for scientific computing: plotting, data analisys, parallelization, ...

Why Python? Batteries Included

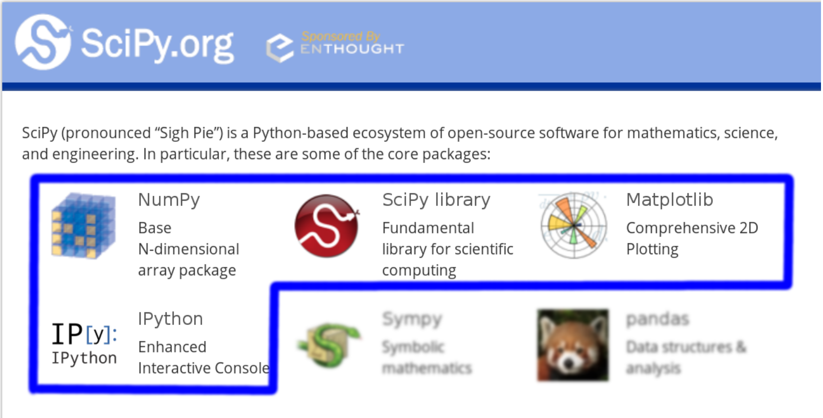
Python Scientific Computing Environment

SciPy.org Sponsored By ENTHOUGHT

SciPy (pronounced "Sigh Pie") is a Python-based ecosystem of open-source software for mathematics, science, and engineering. In particular, these are some of the core packages:

NumPy Base N-dimensional array package	**SciPy library** Fundamental library for scientific computing	**Matplotlib** Comprehensive 2D Plotting
IPython Enhanced Interactive Console	**Sympy** Symbolic mathematics	**pandas** Data structures & analysis

Python Scientific Computing Environment



NumPy

NumPy is the fundamental package for scientific computing with Python. It contains among other things:

- a powerful N-dimensional array object
- sophisticated (broadcasting) functions
- tools for integrating C/C++ and Fortran code
- useful linear algebra, Fourier transform, and random number capabilities

NumPy

NumPy
Base
N-dimensional
array package

SciPy library
Fundamental
library for scientific
computing

Matplotlib
Comprehensive 2D
Plotting

IPython
Enhanced
Interactive Console

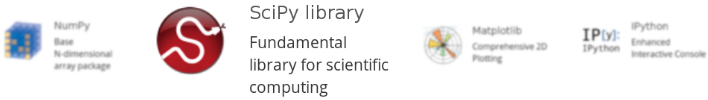
```
import numpy as np

# Create a numpy array, x
X = np.array( [1.1, 1.3, 1.5] )
y = np.sin(a)

# create a random two dimensional numpy array, A
A = np.random.rand(3,3)

A.transpose()
A.trace()
```

SciPy



SciPy is a collection of mathematical algorithms and convenience functions built on the Numpy extension of Python.

Provides the user with high-level commands and classes for manipulating and visualizing data.

With SciPy an interactive Python session becomes a data-processing and system-prototyping environment rivaling sytems such as MATLAB, IDL, Octave, R-Lab, and SciLab.

SciPy

NumPy
Base
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SciPy subpackages (some of them)

- constants: Physical and mathematical constants
- fftpack: Fast Fourier Transform routines
- integrate: Integration and ordinary differential equation solvers
- interpolate: Interpolation and smoothing splines
- linalg: Linear algebra
- optimize: Optimization and root-finding
- signal: Signal processing
- special: Special functions
- ...

SciPy

SciPy library

Fundamental library for scientific computing

```
import numpy as np
from scipy.special import gamma

x = np.array( [1.1, 2., 3.] )
y = gamma(x)

print (y)
```

```
[ 0.95135077,  1. ,  2. ]
```

matplotlib

NumPy Base N-dimensional array package

SciPy library Fundamental library for scientific computing

Matplotlib Comprehensive 2D Plotting

IPython Enhanced Interactive Console

matplotlib is a Python 2D plotting library which produces publication quality figures in a variety of hardcopy formats and interactive environments across platforms.

matplotlib can be used in Python scripts, the Python and IPython shell (ala MATLAB® or Mathematica®), web application servers, and several graphical user interface toolkits.

For simple plotting the `pyplot` interface provides a MATLAB-like interface, particularly when combined with the `IPython / Jupyter` environment.

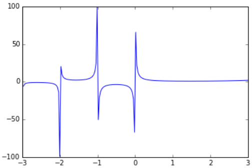
SciPy

Matplotlib
Comprehensive 2D Plotting

```
import numpy as np
from scipy.special import gamma
import matplotlib.pyplot as plt

x = np.linspace( start=-3., stop
    =3., num=200 )
y = gamma(x)

plt.plot(x,y)
plt.savefig("gamma.png")
```



SciPy

Matplotlib
Comprehensive 2D Plotting

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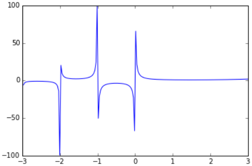


Just google matplotlib images for examples!

IPython / Jupyter

IPython
Enhanced
Interactive Console

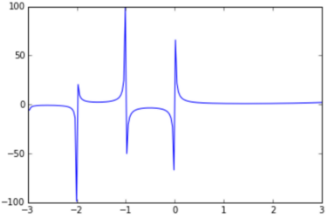
The **IPython / Jupyter Notebook** is a web-based interactive computing system that enables users to author documents that include live code, narrative text, LaTeXequations, HTML, images and video.

These documents contain a full record of a computation and its results and can be shared on email, Dropbox, version control systems (like git/GitHub) or with the Jupyter online notebook viewer nbviewer.jupyter.org.

IPython / Jupyter

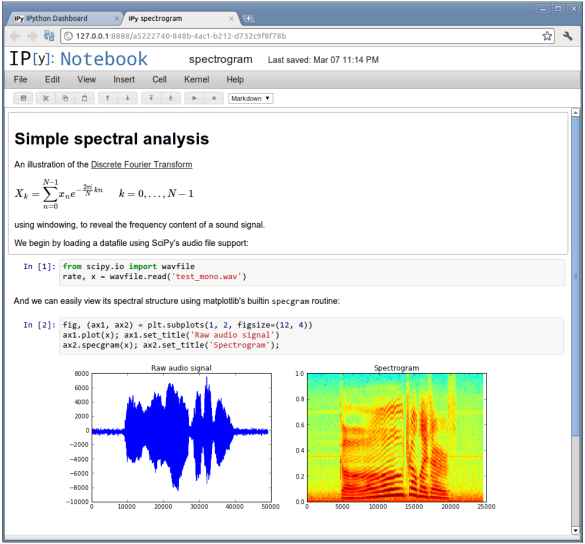
In [45]:
```
%matplotlib inline
import numpy as np
from scipy.special import gamma
import matplotlib.pyplot as plt

x = np.linspace( start=-3., stop=3., num=200 )
y = gamma(x)

plt.plot(x,y)
```

Out[45]: [<matplotlib.lines.Line2D at 0x7fc4ac4660b8>]



In [ ]:

IPython


IPython Dashboard
spectrogram
127.0.0.1:8888/a5222740-848b-4ac1-b212-d732c9f8f78b
IP[y]: Notebook
spectrogram
Last saved: Mar 07 11:14 PM
File
Edit
View
Insert
Cell
Kernel
Help
Markdown
Simple spectral analysis
An illustration of the Discrete Fourier Transform
$X_k = \sum_{n=0}^{N-1} x_n e^{-\frac{2\pi i}{N} kn} \qquad k = 0, \dots, N-1$
using windowing, to reveal the frequency content of a sound signal.
We begin by loading a datafile using SciPy's audio file support:
In [1]: from scipy.io import wavfile
rate, x = wavfile.read('test_mono.wav')
And we can easily view its spectral structure using matplotlib's builtin specgram routine:
In [2]: fig, (ax1, ax2) = plt.subplots(1, 2, figsize=(12, 4))
ax1.plot(x); ax1.set_title('Raw audio signal')
ax2.specgram(x); ax2.set_title('Spectrogram');
Raw audio signal
Spectrogram

Python Scientific Computing Environment

Let's try it!